Sepp Hochreiter

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Improving Few- and Zero-Shot Reaction Template Prediction Using Modern Hopfield Networks. Journal of Chemical Information and Modeling, 2022, 62, 2111-2120.	5.4	30
2	Domain Shifts in Machine Learning Based Covid-19 Diagnosis From Blood Tests. Journal of Medical Systems, 2022, 46, 23.	3.6	14
3	Uncertainty estimation with deep learning for rainfall–runoff modeling. Hydrology and Earth System Sciences, 2022, 26, 1673-1693.	4.9	38
4	In silico proof of principle of machine learning-based antibody design at unconstrained scale. MAbs, 2022, 14, 2031482.	5.2	40
5	Artificial neural networks and pathologists recognize basal cell carcinomas based on different histological patterns. Modern Pathology, 2021, 34, 895-903.	5.5	20
6	The Promise of AI for DILI Prediction. Frontiers in Artificial Intelligence, 2021, 4, 638410.	3.4	31
7	Rainfall–runoff prediction at multiple timescales with a single Long Short-Term Memory network. Hydrology and Earth System Sciences, 2021, 25, 2045-2062.	4.9	106
8	A note on leveraging synergy in multiple meteorological data sets with deep learning for rainfall–runoff modeling. Hydrology and Earth System Sciences, 2021, 25, 2685-2703.	4.9	35
9	Quantum Optical Experiments Modeled by Long Short-Term Memory. Photonics, 2021, 8, 535.	2.0	7
10	Machine learning–based prediction of transfusion. Transfusion, 2020, 60, 1977-1986.	1.6	22
11	Industry-scale application and evaluation of deep learning for drug target prediction. Journal of Cheminformatics, 2020, 12, 26.	6.1	23
12	Cost Optimization at Early Stages of Design Using Deep Reinforcement Learning. , 2020, , .		2
13	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. Nature Communications, 2019, 10, 2674.	12.8	240
14	Accurate Prediction of Biological Assays with High-Throughput Microscopy Images and Convolutional Networks. Journal of Chemical Information and Modeling, 2019, 59, 1163-1171.	5.4	69
15	Machine Learning in Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 945-946.	5.4	43
16	On failure modes in molecule generation and optimization. Drug Discovery Today: Technologies, 2019, 32-33, 55-63.	4.0	59
17	Towards learning universal, regional, and local hydrological behaviors via machine learning applied to large-sample datasets. Hydrology and Earth System Sciences, 2019, 23, 5089-5110.	4.9	276
18	Toward Improved Predictions in Ungauged Basins: Exploiting the Power of Machine Learning. Water Resources Research, 2019, 55, 11344-11354.	4.2	279

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19	Explaining and Interpreting LSTMs. Lecture Notes in Computer Science, 2019, , 211-238.	1.3	44
20	Visual Scene Understanding for Autonomous Driving Using Semantic Segmentation. Lecture Notes in Computer Science, 2019, , 285-296.	1.3	21
21	Interpretable Deep Learning in Drug Discovery. Lecture Notes in Computer Science, 2019, , 331-345.	1.3	62
22	NeuralHydrology – Interpreting LSTMs in Hydrology. Lecture Notes in Computer Science, 2019, , 347-362.	1.3	46
23	Repurposing High-Throughput Image Assays Enables Biological Activity Prediction for Drug Discovery. Cell Chemical Biology, 2018, 25, 611-618.e3.	5.2	176
24	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. Bioinformatics, 2018, 34, 1538-1546.	4.1	341
25	Fréchet ChemNet Distance: A Metric for Generative Models for Molecules in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 1736-1741.	5.4	161
26	Machine Learning in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 1723-1724.	5.4	21
27	Large-scale comparison of machine learning methods for drug target prediction on ChEMBL. Chemical Science, 2018, 9, 5441-5451.	7.4	357
28	panelcn.MOPS: Copy-number detection in targeted NGS panel data for clinical diagnostics. Human Mutation, 2017, 38, 889-897.	2.5	72
29	Rectified factor networks for biclustering of omics data. Bioinformatics, 2017, 33, i59-i66.	4.1	7
30	IBD Sharing between Africans, Neandertals, and Denisovans. Genome Biology and Evolution, 2016, 8, 3406-3416.	2.5	6
31	DeepTox: Toxicity Prediction using Deep Learning. Frontiers in Environmental Science, 2016, 3, .	3.3	593
32	Prediction of human population responses to toxic compounds by a collaborative competition. Nature Biotechnology, 2015, 33, 933-940.	17.5	88
33	Using transcriptomics to guide lead optimization in drug discovery projects: Lessons learned from the QSTAR project. Drug Discovery Today, 2015, 20, 505-513.	6.4	80
34	Rchemcpp: a web service for structural analoging in ChEMBL, Drugbank and the Connectivity Map. Bioinformatics, 2015, 31, 3392-3394.	4.1	16
35	KeBABS: an R package for kernel-based analysis of biological sequences. Bioinformatics, 2015, 31, 2574-2576.	4.1	44
36	msa: an R package for multiple sequence alignment. Bioinformatics, 2015, 31, 3997-3999.	4.1	458

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37	Connecting gene expression data from connectivity map and in silico target predictions for small molecule mechanism-of-action analysis. Molecular BioSystems, 2015, 11, 86-96.	2.9	28
38	Assessing technical performance in differential gene expression experiments with external spike-in RNA control ratio mixtures. Nature Communications, 2014, 5, 5125.	12.8	122
39	A comprehensive assessment of RNA-seq accuracy, reproducibility and information content by the Sequencing Quality Control Consortium. Nature Biotechnology, 2014, 32, 903-914.	17.5	883
40	Furby: fuzzy force-directed bicluster visualization. BMC Bioinformatics, 2014, 15, S4.	2.6	38
41	HapFABIA: Identification of very short segments of identity by descent characterized by rare variants in large sequencing data. Nucleic Acids Research, 2013, 41, e202-e202.	14.5	21
42	DEXUS: identifying differential expression in RNA-Seq studies with unknown conditions. Nucleic Acids Research, 2013, 41, e198-e198.	14.5	26
43	Increasing the discovery power of -omics studies. Systems Biomedicine (Austin, Tex), 2013, 1, 84-93.	0.7	2
44	cn.MOPS: mixture of Poissons for discovering copy number variations in next-generation sequencing data with a low false discovery rate. Nucleic Acids Research, 2012, 40, e69-e69.	14.5	394
45	Genome-Wide Chromatin Remodeling Identified at GC-Rich Long Nucleosome-Free Regions. PLoS ONE, 2012, 7, e47924.	2.5	13
46	APCluster: an R package for affinity propagation clustering. Bioinformatics, 2011, 27, 2463-2464.	4.1	407
47	cn.FARMS: a latent variable model to detect copy number variations in microarray data with a low false discovery rate. Nucleic Acids Research, 2011, 39, e79-e79.	14.5	19
48	Complex Networks Govern Coiled-Coil Oligomerization – Predicting and Profiling by Means of a Machine Learning Approach. Molecular and Cellular Proteomics, 2011, 10, M110.004994.	3.8	39
49	Detection of Nonlinear Effects in Gene Expression Pathways. Nature Precedings, 2010, , .	0.1	0
50	Identifying Copy Number Variations based on Next Generation Sequencing Data by a Mixture of Poisson Model. Nature Precedings, 2010, , .	0.1	0
51	Informative or Noninformative Calls for Gene Expression: A Latent Variable Approach. Statistical Applications in Genetics and Molecular Biology, 2010, 9, Article 4.	0.6	8
52	Filtering data from high-throughput experiments based on measurement reliability. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, E173-4; author reply E175.	7.1	21
53	FABIA: factor analysis for bicluster acquisition. Bioinformatics, 2010, 26, 1520-1527.	4.1	258
54	An SMO Algorithm for the Potential Support Vector Machine. Neural Computation, 2008, 20, 271-287.	2.2	27

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55	I/NI-calls for the exclusion of non-informative genes: a highly effective filtering tool for microarray data. Bioinformatics, 2007, 23, 2897-2902.	4.1	154
56	Fast model-based protein homology detection without alignment. Bioinformatics, 2007, 23, 1728-1736.	4.1	106
57	Optimality of LSTD and its Relation to MC. , 2007, , .		1
58	Monaural Speech Separation by Support Vector Machines: Bridging the Divide Between Supervised and Unsupervised Learning Methods. Signals and Communication Technology, 2007, , 411-428.	0.5	1
59	A new summarization method for affymetrix probe level data. Bioinformatics, 2006, 22, 943-949.	4.1	229
60	Support Vector Machines for Dyadic Data. Neural Computation, 2006, 18, 1472-1510.	2.2	73
61	Nonlinear Feature Selection with the Potential Support Vector Machine. Studies in Fuzziness and Soft Computing, 2006, , 419-438.	0.8	11
62	Learning to Learn Using Gradient Descent. Lecture Notes in Computer Science, 2001, , 87-94.	1.3	227
63	Feature Extraction Through LOCOCODE. Neural Computation, 1999, 11, 679-714.	2.2	55
64	The Vanishing Gradient Problem During Learning Recurrent Neural Nets and Problem Solutions. International Journal of Uncertainty, Fuzziness and Knowlege-Based Systems, 1998, 06, 107-116.	1.9	1,725
65	LOCOCODE versus PCA and ICA. Perspectives in Neural Computing, 1998, , 669-674.	0.1	3
66	Flat Minima. Neural Computation, 1997, 9, 1-42.	2.2	388
67	Unsupervised coding with lococode. Lecture Notes in Computer Science, 1997, , 655-660.	1.3	4
68	Long Short-Term Memory. Neural Computation, 1997, 9, 1735-1780.	2.2	58,553
69	Optimal gradient-based learning using importance weights. , 0, , .		1
70	Optimal kernels for unsupervised learning. , 0, , .		0
71	Large-Scale Ligand-Based Virtual Screening for SARS-CoV-2 Inhibitors Using Deep Neural Networks. SSRN Electronic Journal, 0, , .	0.4	35